# Modeling an Iodine Hall Thruster Plume in the Iodine Satellite (iSAT)

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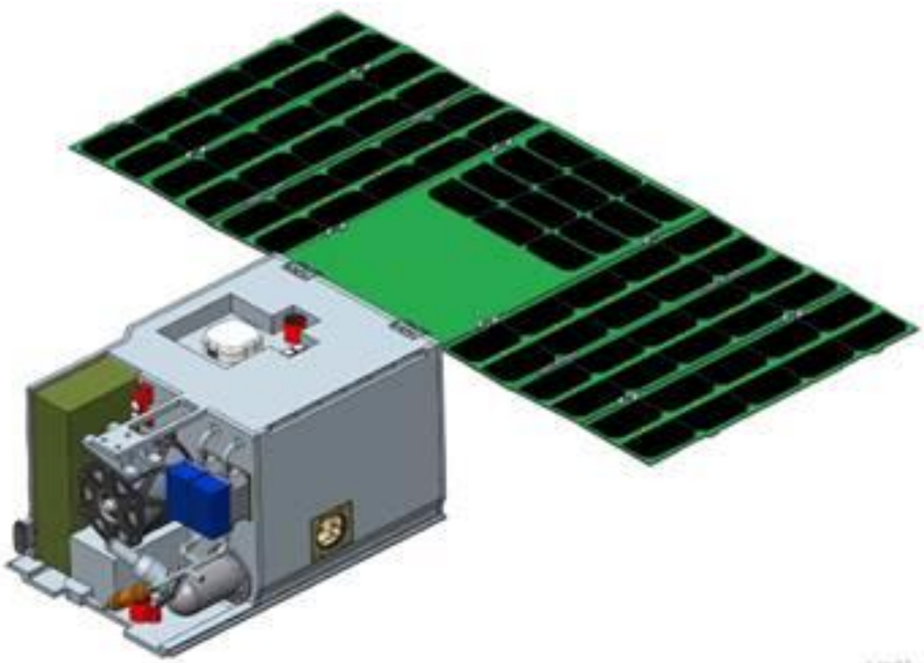
# Using Iodine for Hall-Effect Thrusters (HETs)

- Iodine has been identified as an attractive alternative propellant to Xe for HETs
  - High storage density (2-3 times of Xe)
  - Efficient ionization (lower ionization potential, higher ionization cross section than Xe)
  - Similar mass for I and larger mass for $I_2$ than Xe
  - Comparable performance to Xe with higher T/P ratio at higher power operating condition
- A dearth of detailed knowledge of physical processes occurring in the plume
- Critical risk: High reactivity
  - Concern for spacecraft system integration

# OBJECTIVE

- Simulate the iodine plasma plume generated by BHT-200 Hall thruster and its interaction with the spacecraft body/solar array in the iSAT

**Busek's BHT-200 Thruster**



**Basic configuration of iSAT**

# OVERVIEW OF NUMERICAL MODEL

- 3-D Hybrid-particle code, DRACO, developed at AFRL
  - Particle-in-cell (PIC) combined with Monte Carlo Collision (MCC)
- Quasi-neutrality
- Boltzmann relation with a polytropic temperature model:

$$\phi = \phi_r + \frac{k_B T_{e,r}}{e}\left(\frac{\gamma}{\gamma - 1}\right)\left[\left(\frac{n_e}{n_{e,r}}\right)^{\gamma-1} - 1\right]$$

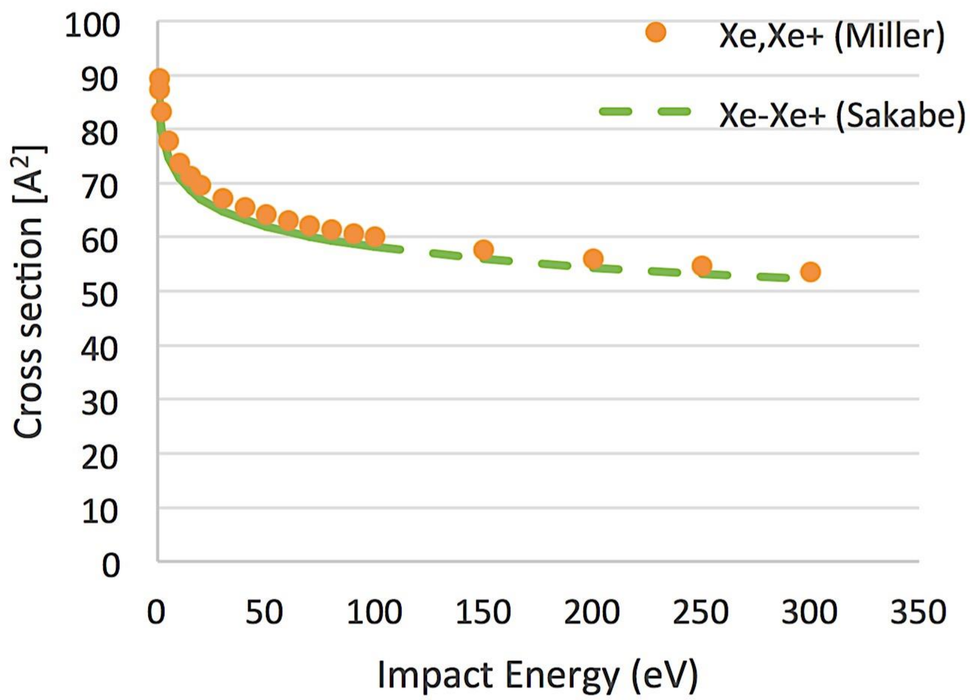
# Collision cross section models (1)

- Neutral-neutral: Momentum-exchange (MEX)
  - Variable Hard-Sphere model
- Ion-neutral: Momentum- and charge-exchange (CEX)
  - Semi-empirical models based on measurements
- For iodine, CEX collision is also important in a Hall thruster plume
  - Consider: $I\text{-}I^+$, $I_2\text{-}I^+$, and $I_2\text{-}I_2^+$
    - $I_2\text{-}I^+$, and $I_2\text{-}I_2^+$ available from measurement[1]
    - $I\text{-}I^+$ calculated using Sakabe's formula[2]

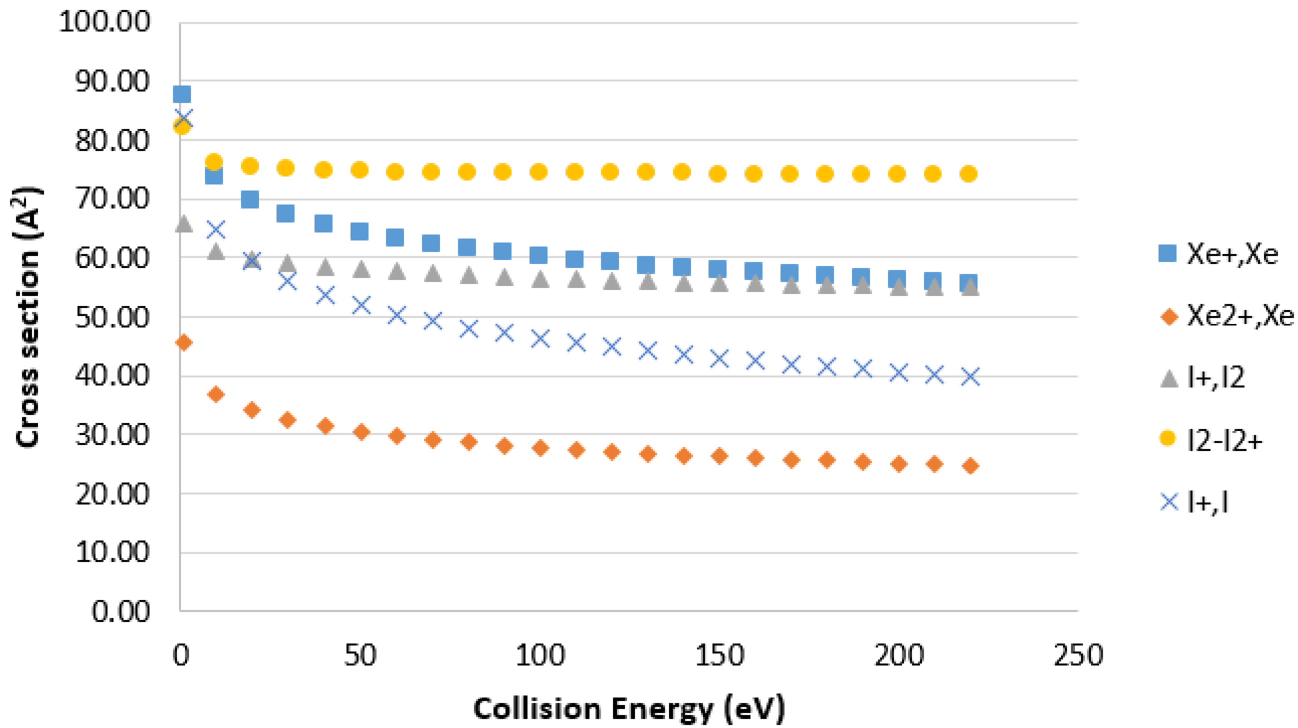
[1] M. L. Hause, B. D. Prince and R. J. Bemish, "A guided-ion beam study of the collisions and reactions of I+ and I2+ with I2," *The Journal of Chemical Physics,* vol. 142, no. 7, 2015.
[2] S. Sakabe and Y. Izawa, "Simple formula for the cross sections of resonant charge transfer between atoms and their positive ions at low impact velocity," Physical Review A, vol. 45, no. 3, p. 2086, 1 February 1992.

# Collision cross section models (2)

- Verify Sakabe's formula using Xe-$Xe^+$ data by Miller



# COLLISION CROSS SECTION MODELS (3)




$$\sigma_{CEX} = A - B\,log(E)$$

| | A | B |
|---|---|---|
| **Xe-Xe$^+$** | 87.3 | 13.6 |
| **Xe-Xe$^+$** | 45.7 | 8.9 |
| **$I_2$-I$^+$** | 66.0 | 4.7 |

$I_2$-$I_2$$^+$:

$$\sigma_{CEX}(I^+, I_2) = c_1 \log^3(E) + c_2 \log^2(E) + c_3 \log^1(E) + c_4$$

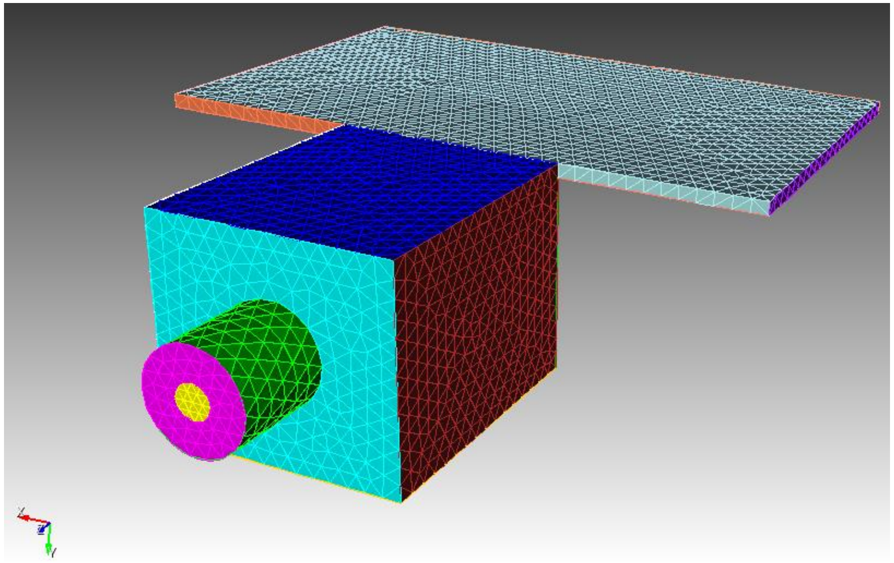
| $c_1$ | $c_2$ | $c_3$ | $c_4$ |
|---|---|---|---|
| -0.47 | 3.5 | -9.0 | 82.0 |

I-I$^+$:

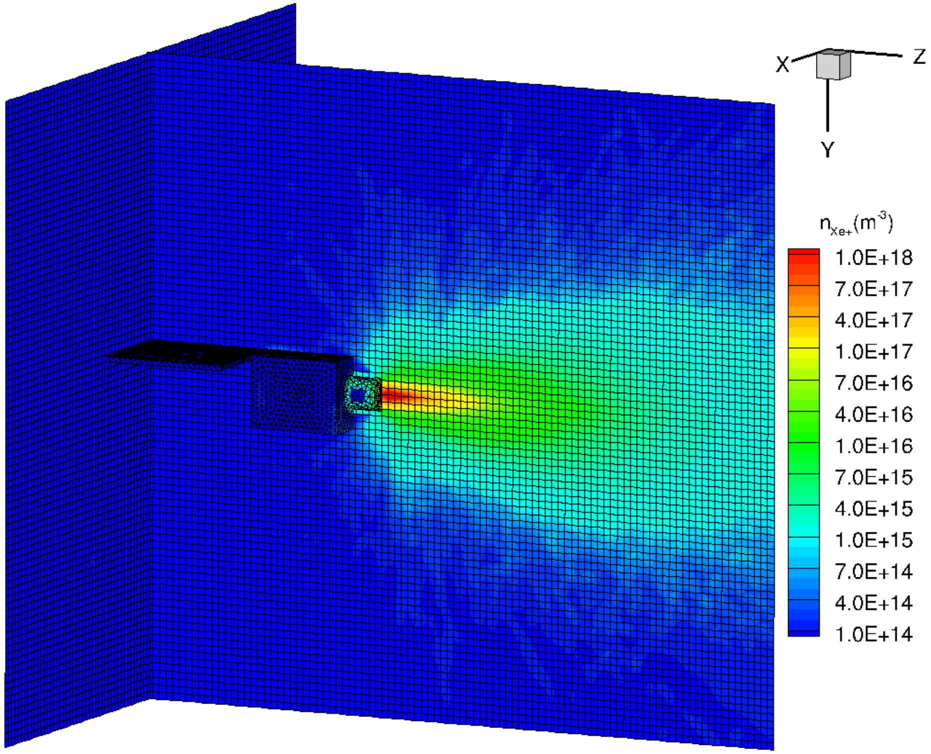
$$\sigma(v) = [A - B\,log_{10}(v)]\left(\frac{\varepsilon_I}{\varepsilon_{I_0}}\right)^{-1.5}$$

$$A = 1.81 \times 10^{-14}$$
$$B = 2.12 \times 10^{-15}$$
$$\varepsilon_{I_0} = 13.6\,\mathrm{eV}$$

# SURFACE & VOLUME MESH



Create the geometry & surface meshing in Cubit




Create the volume mesh using Volcar

# PARAMETERS USED FOR SIMULATION

| | Xenon | Iodine |
|---|---|---|
| Discharge voltage (V) | 250 | 250 |
| Discharge current (A) | 0.75 | 0.74 |
| Anode mass flow rate (mg/s) | 0.84 | 0.82 |
| Cathode mass flow rate (mg/s) | 0.098 | 0.096 |
| Mass (propellant) utilization efficiency | 0.981 | 0.853 |
| Ion mass flow rate (kg/s) | 8.24E-07 | 6.99E-07 |
| Species temperature (K) | 700 | 700 |

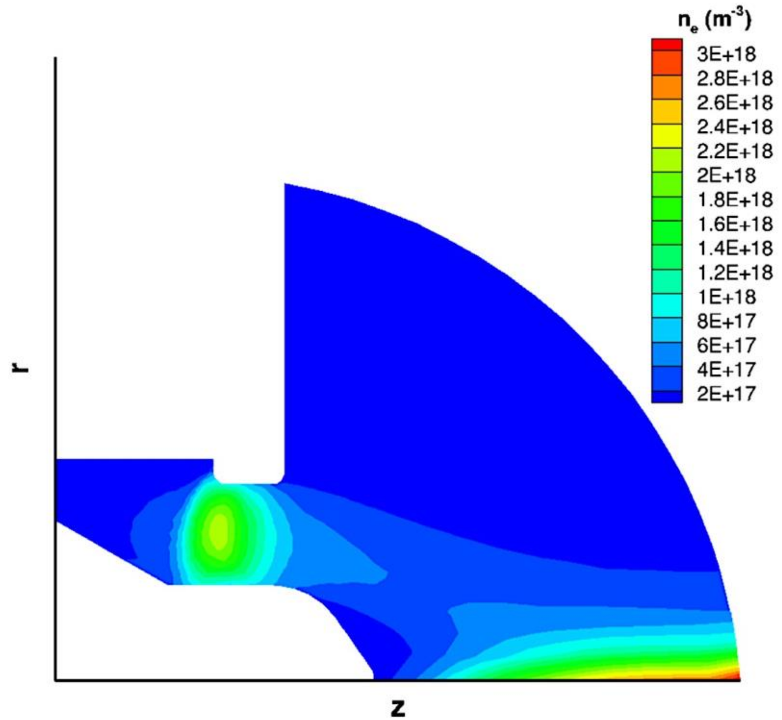

[3] Nakles, M. R., Brieda, L.., Reed, G. D., Hargus, W. A., and Spicer, R. L., "Experimental and numerical examination of the BHT-200 hall thruster plume," 43rd AIAA/ASME/SAE/ASEE Joint Propulsion Conference & Exhibit, 8-11 July 2007, Cincinnati, OH, AIAA-2007-5305.

[4] Hillier, Adam C. *Revolutionizing space propulsion through the characterization of iodine as fuel for hall-effect thrusters*. No. AFIT/GA/ENY/11-M08. AIR FORCE INST OF TECH WRIGHT-PATTERSON AFB OH GRADUATE SCHOOL OF ENGINEERING AND MANAGEMENT, 2011.

[5] Szabo, J., Pote, B., Paintal, S., Robin, M., Hillier, A., Branam, R. D., and Huffmann, R. E., "Performance evaluation of an iodine-vapor Hall thruster." *Journal of Propulsion and Power* 28, no. 4 (2012): 848-857.

# Simulation of Xenon

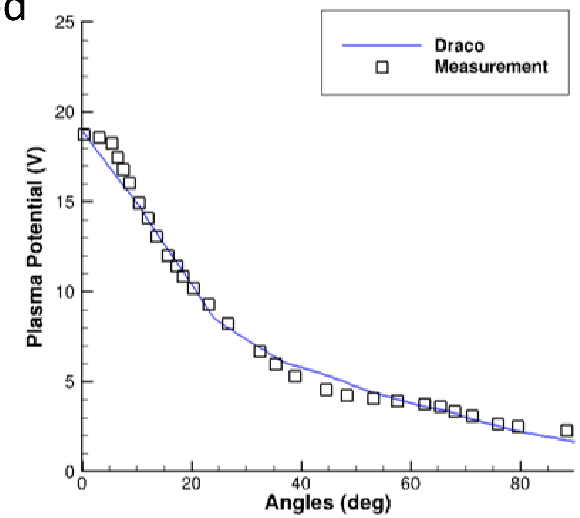
- Use HPHall source to provide particle information
- Compare with measurement by Nakles (2007)
  - Facility backpressure: $5 \times 10^{-6}$ Torr $\approx 1.6 \times 10^{17}\ m^{-3}$



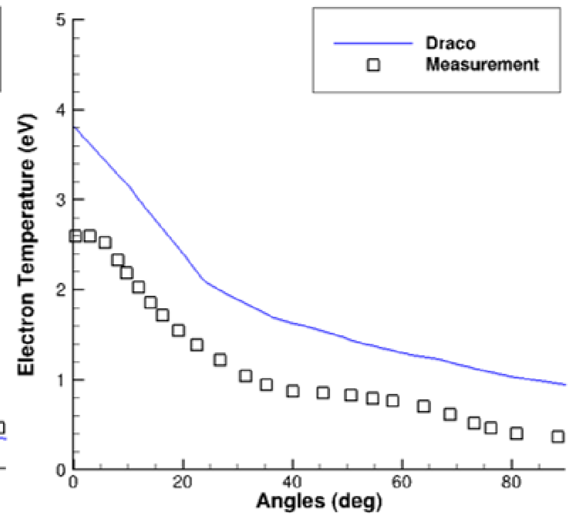
# COMPARISON WITH EXPERIMENTAL DATA

- Generally good agreement

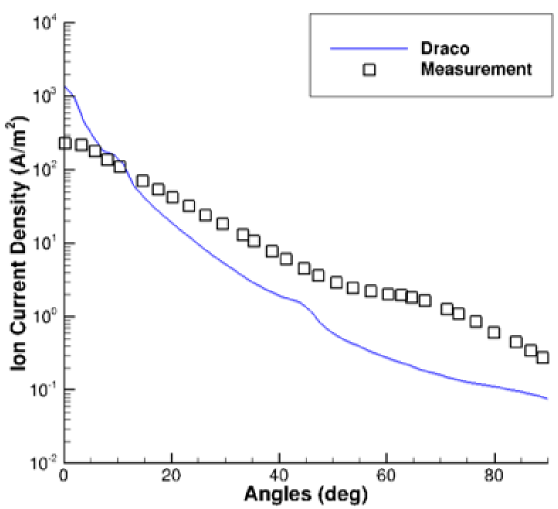
## Plasma Potential



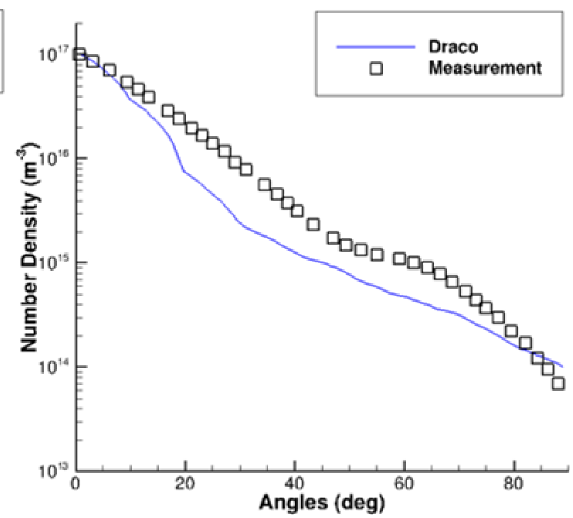

## Electron Temperature




## Ion Current Flux




## Ion Number Density

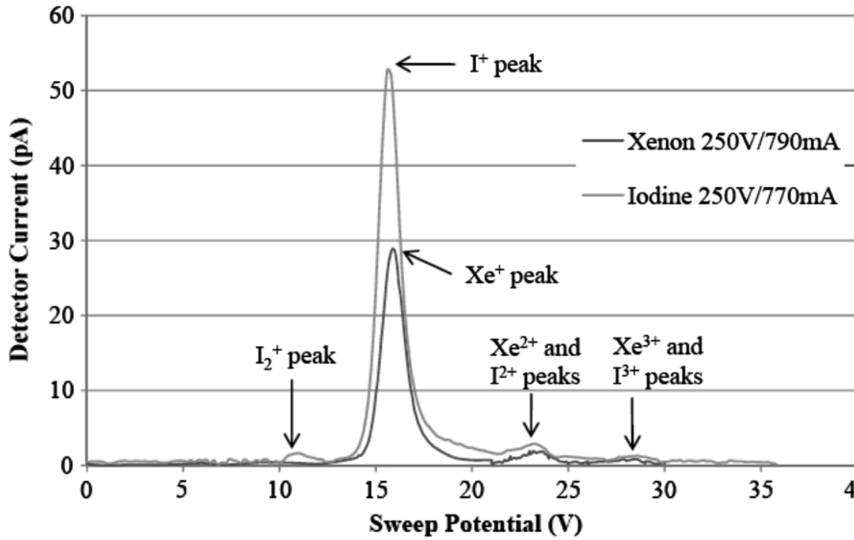


# SIMULATION OF IODINE PLUME (1)

- Additional reactions due to molecular species ($I_2$, and $I_2^+$)
  - Including dissociative ionization, electron attachment, and inelastic energy exchange
- Accurate modeling requires these processes to be implemented in the model
  - However, the goal is to provide a first-order approximation of the iodine particle flux on spacecraft surfaces using the numerical tools available to us at this stage
- Atomic iodine species ($I$, $I^+$, and $I^{2+}$) are simulated using the HPHall
- Molecular species are introduced at the discharge channel exit assuming Maxwellian velocity distributions.

# SIMULATION OF IODINE (2)

- Use iodine mole fraction measurement and mass utilization efficiency 85.3% to calculate $I_2$ and $I_2^+$ mass flow rates
  - Assumed 10% of the total neutral flow is $I_2$

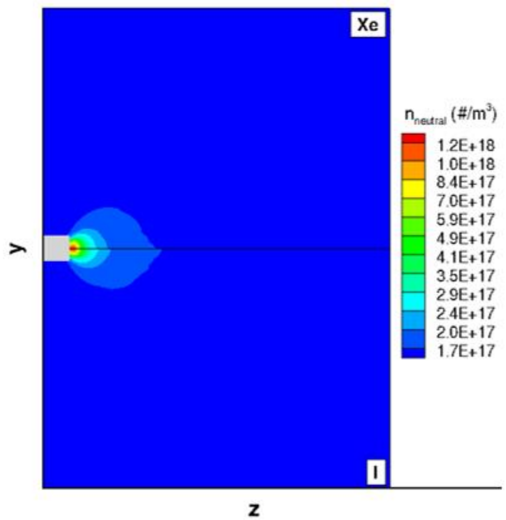



| Species | Mole Fraction, Xe | Mole Fraction, I |
|---|---|---|
| $I_2^+$ | | 0.029 |
| $Xe^+, I^+$ | 0.975 | 0.953 |
| $Xe^{2+}, I^{2+}$ | 0.021 | 0.015 |
| $Xe^{3+}, I^{3+}$ | 0.004 | 0.003 |

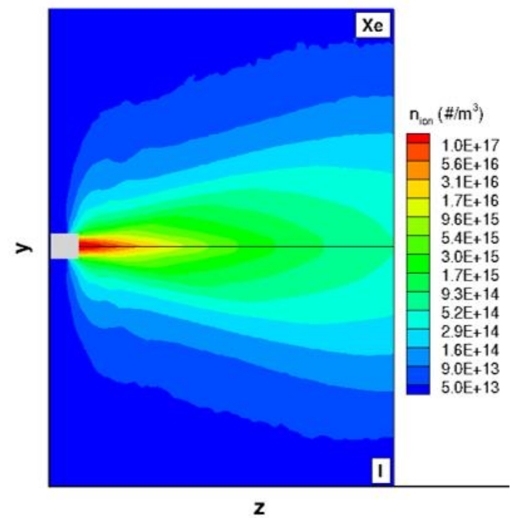
# XENON VS IODINE

- Similar result between Xe vs. I

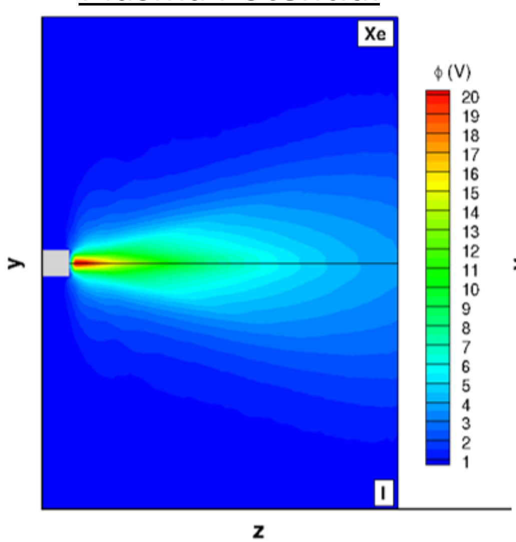
### Neutral Number Density



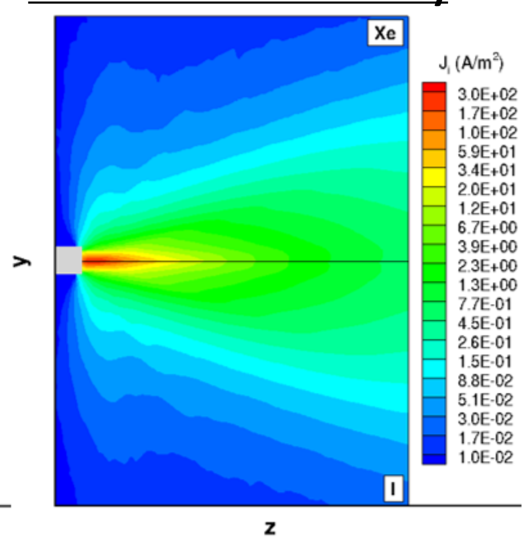

### Ion Number Density




### Plasma Potential



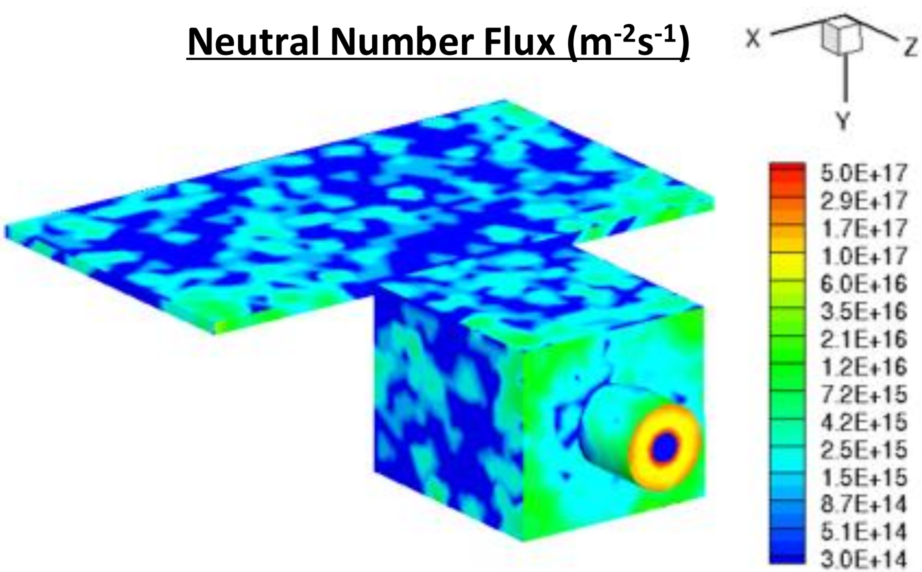

### Neutral Current Density



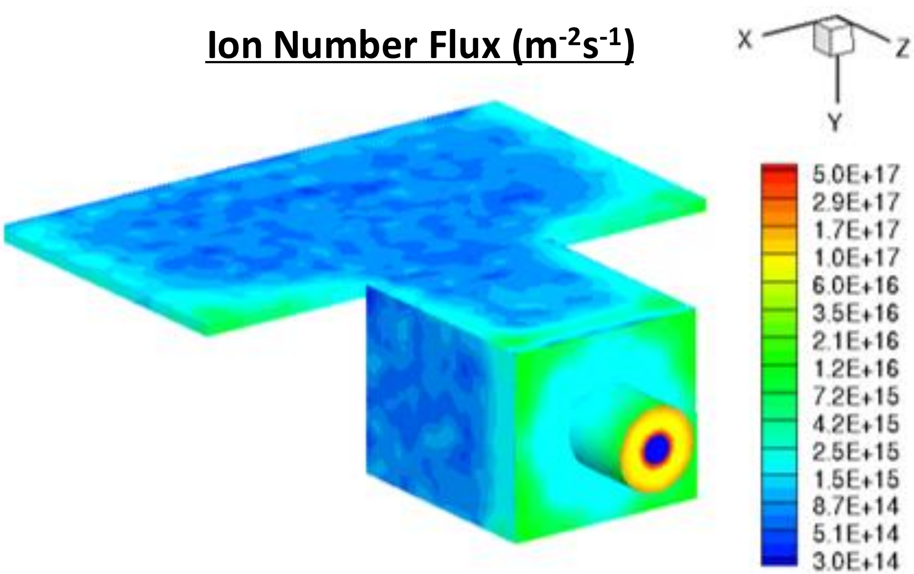
# ESTIMATE OF IODINE FLUX ON SURFACE

- Fluxes decrease away from the thruster in general
- Higher flux on outer edge of the front surface of s/c body and solar array
- Highest total iodine flux on the solar array: $4.5 \times 10^{16}$ $m^{-2}s^{-1}$
- Deposition per unit area: 0.34 $mg/cm^2$ over the entire thruster operation duration assuming 100% deposits

**Neutral Number Flux ($m^{-2}s^{-1}$)**




**Ion Number Flux ($m^{-2}s^{-1}$)**



# SUMMARY & CONCLUSIONS

- Verified the model using Xe data
- Simulated iodine plume with the mass flow rates based on experimental data
- Deposition per unit area: 0.34 mg/cm$^2$ over the entire thruster operation duration assuming 100% deposits
- In reality, only some portion of iodine colliding with the surface may chemically react with the surface
- How many particles actually react to or reflect off the surface will depend on the surface properties of the solar panel
- For more physically accurate simulation of iodine plasma plume, one needs to model the detailed reactions, especially the dissociative ionization

# ACKNOWLEDGEMENT

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